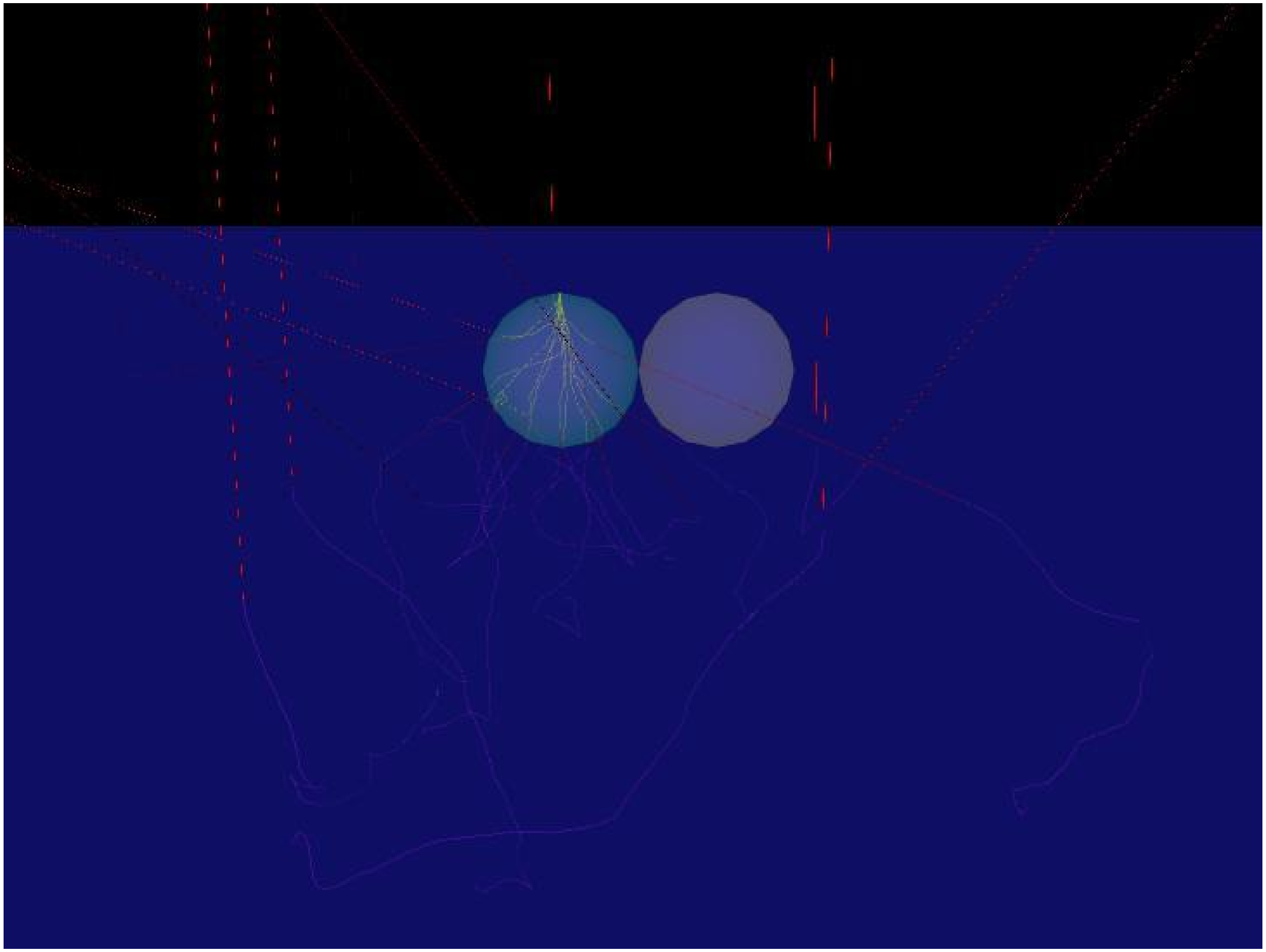
Studying Particle Proximity in VP Microanalysis using NISTMonte

Nicholas W. M. Ritchie
National Institute of Standards and Technology
Gaithersburg, MD

Question:

How does a proximate particle effect microanalysis in a low-vacuum SEM?



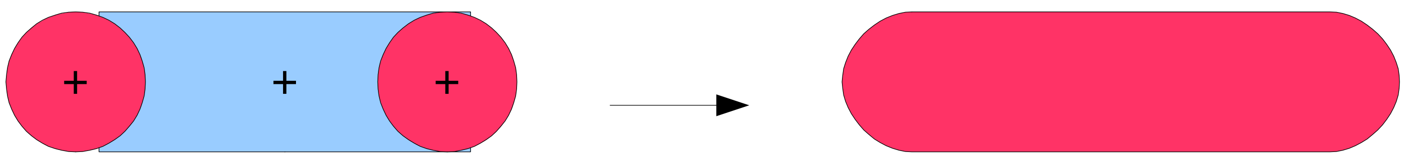
Consider two particles of different composition on a carbon substrate analyzed in H_2O vapor.

Introduction to NISTMonte

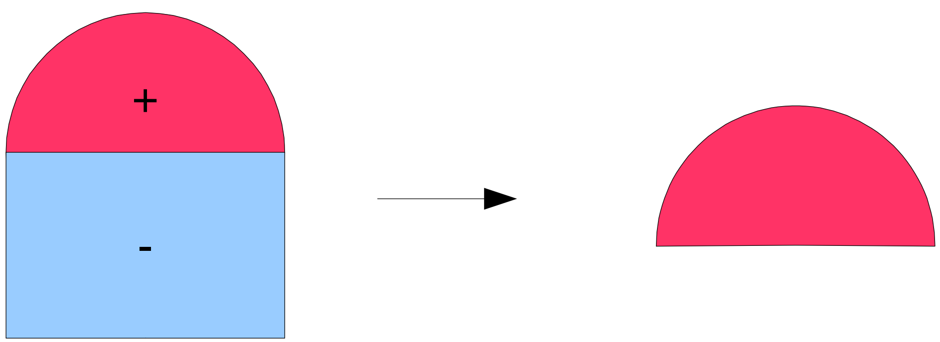
- Monte Carlo simulation of electron transport and x-ray generation and transport
  - Written in Java (J2SE 1.4 or higher)
  - Available with source code
- Features
  - Arbitrarily complex sample geometries
  - Interchangeable physics
  - Mix & match detection schemes
  - Scriptable in Jython, Java or ?

Sample geometries

- Constructed from basic 3D shapes
  - Sphere, Cylinder, Block, Intersection of Planes
- 3D shapes may be combined or differenced
  - 2 spheres + cylinder -> cylinder with rounded ends



  - Sphere - plane -> hemisphere



Interchangeable physics

- Elastic scattering models
  - Screened Rutherford
  - NIST SRM-64 (Jablonski, Salvat & Powell)
  - Czyzweski (Czyzewski, MacCallum, Romig & Joy)
- Mass absorption coefficients
  - NIST FFAST
  - Heinrich IXCOM 11
  - Many more...
- Energy loss models
- Characteristic x-ray generation model

Detection Schemes

- Backscatter
  - Energy resolved backscatter detector
- Annular detector
  - Records electrons passing through a concentric set of planar rings
- X-ray emission image
  - Image per x-ray line showing the spatial dependence of generation and emission
- Trajectory image
  - Showing electron trajectories projected into a plane
- Trajectory VRML
  - Shows sample geometry and electron trajectories in a 3D CAD-like view
- Spectrum generation
  - Models an EDS detector measuring characteristic & bremsstrahlung emission

Scriptable

```
tw=jio.OutputStreamWriter(jio.FileOutputStream(baseDir+"result.csv"),cs.Charset.
forName("UTF-8"))
for pressure in [5.0, 10.0, 30.0, 50.0, 100.0]: # pascal
    print "Pressure = %g Pa" % (pressure)
    # create an instance of the model
    monte = nm.MonteCarloSS()
    monte.setPhysics(nm.VPCompatiblePhysics())
    monte.setBeamEnergy(epq.ToSI.keV(25.0))
    # create a region of N2 above the substrate (15 mm)
    mat = epq.Gas([epq.Element.N],[2], pressure,epq.ToSI.centigrade(25.0), "N2")
    shape = nm.SimpleBlock([width/2.0,width/2.0,-15.0e-3],[-width/2.0,-
width/2.0,0.0])
    vpRegion = monte.addSubRegion(monte.getChamber(),mat, shape)
    # place an annular detector above the primary particle
    annular1 = nm.AnnularDetector(epq.ToSI.micrometer(1000.0), 100,
[0.0,0.0,0.0], [0.0,0.0,-1.0])
    monte.addActionListener(annular1)
    monte.runMutipleTrajectories(10000)
    tw.write("Pressure\t%g Pa\n" % (pressure))
    annular1.dump(tw)
tw.close()
```

Loop over pressure

Initialize the model

Define the geometry

Add detector(s)

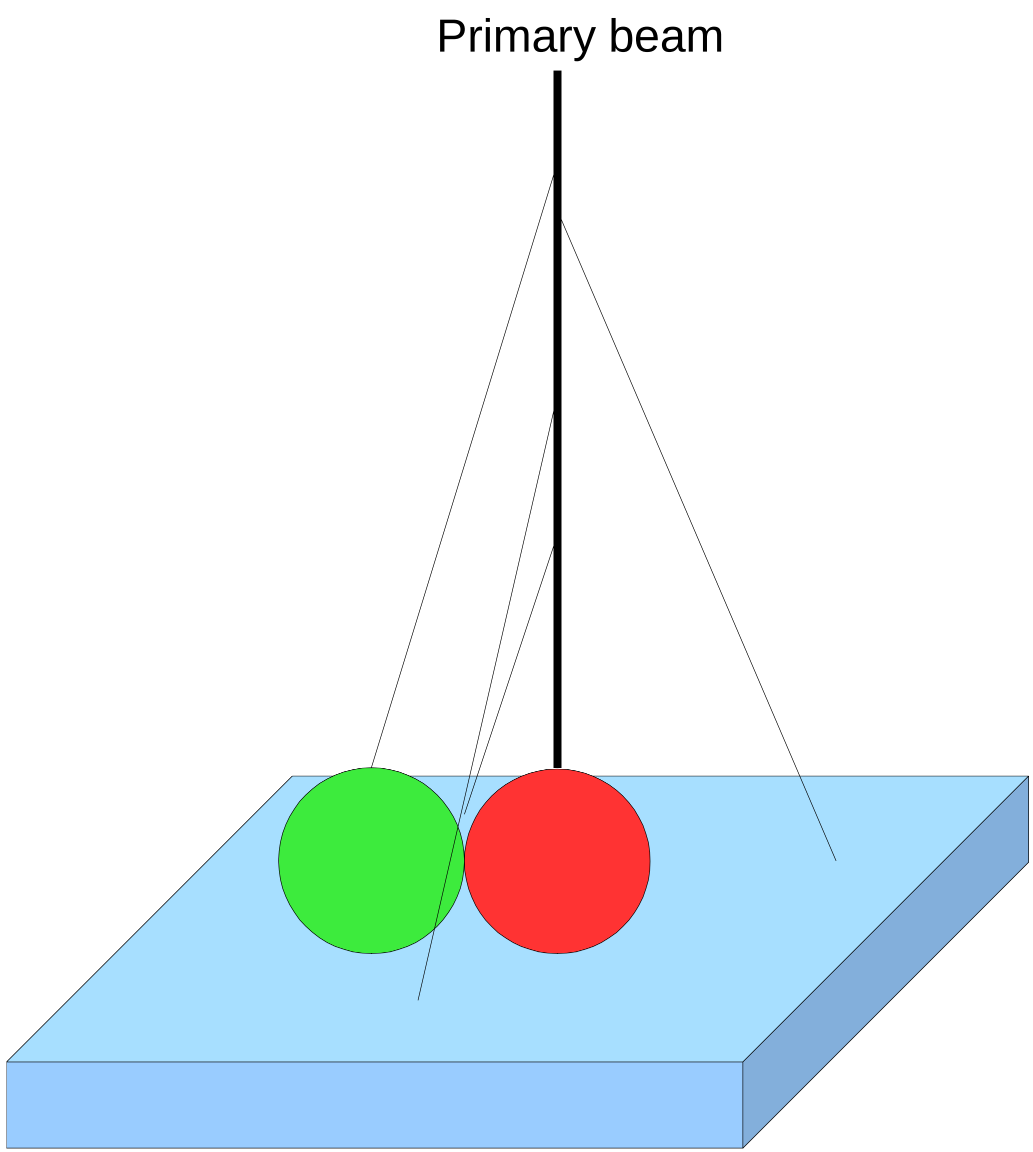
Run the analysis

Write the results

Pro: Flexible, permanent record, iterable
Con: Unintuitive, intimidating to newcomers

Monte Carlo

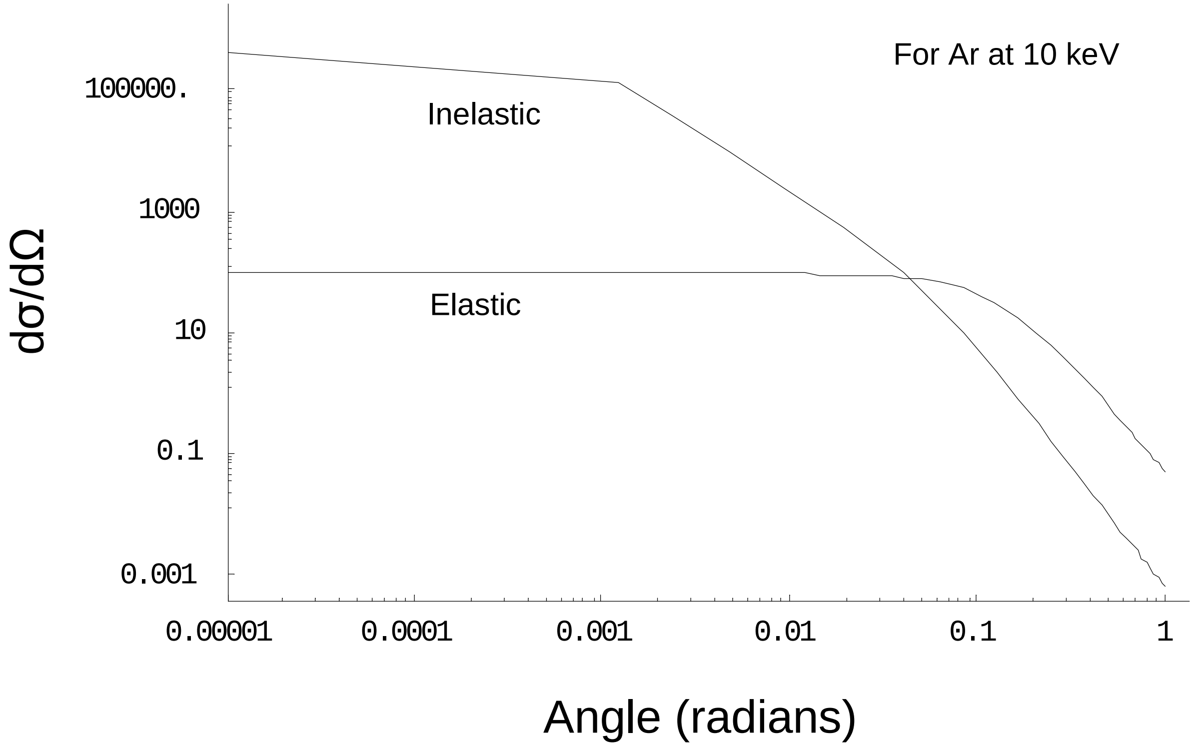
- Standard model
  - Only atomic interactions are considered
    - no molecular or solid state effects are included
  - Only elastic scattering is modeled explicitly
  - Inelastic events are handled on average using a continuously slowing down approximation based on the macroscopic parameter, J, the mean ionization potential
- Adding gas to the model
  - Why not just assume gas is just a diffuse solid?

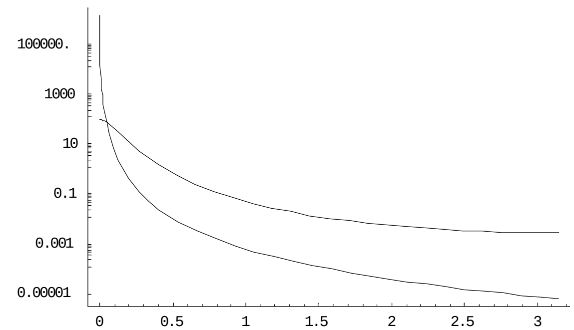

Primary beam

Elastic vs Inelastic Scattering

- Elastic
  - Scattering off of the nucleus (screened by the atomic electrons)
  - Large angular deflection but negligible energy loss
- Inelastic
  - Scattering with energy loss due to multiple atomic and molecular mechanisms
    - Ionization, Excitation (atomic, rotational, vibrational)
  - Smaller angular deflection

Comparing the elastic and inelastic scattering cross sections





Inelastic scattering is strongly peaked in the forward directions.

From Egerton, "Electron Energy-Loss Spectroscopy in the Electron Microscope", Second Edition

Modeling the inelastic cross section

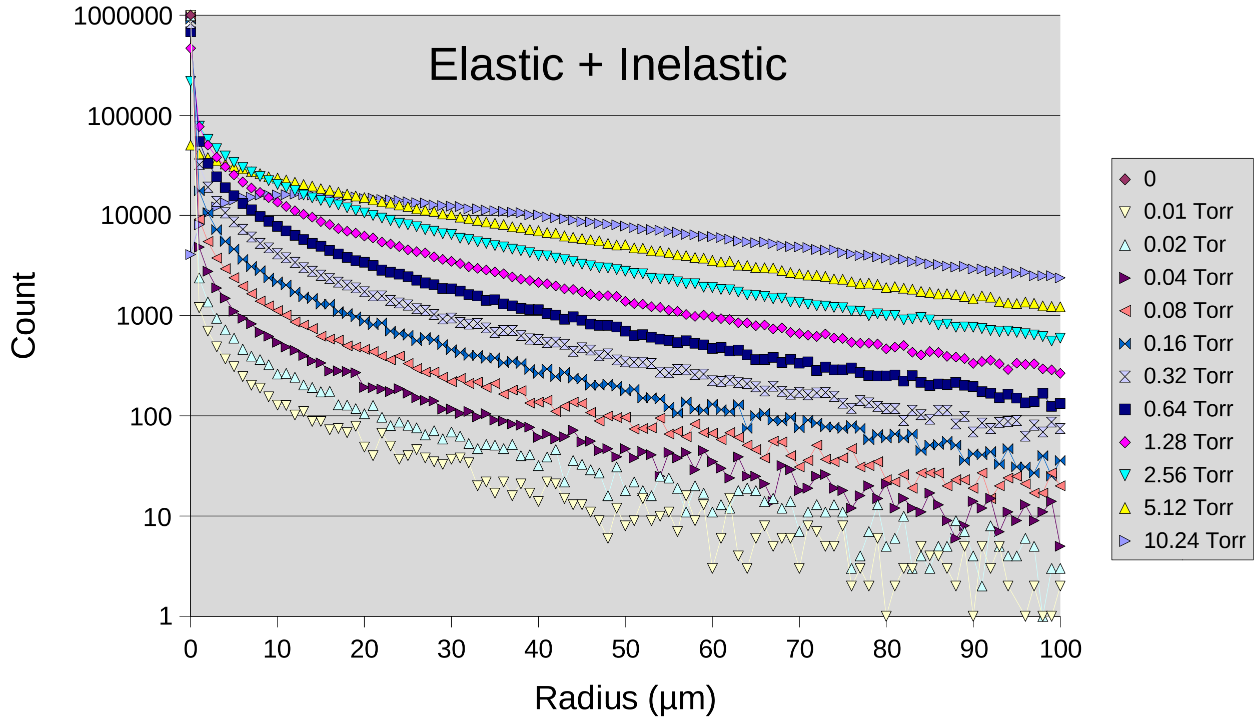
- The magnitude has been observed to scale with atomic number

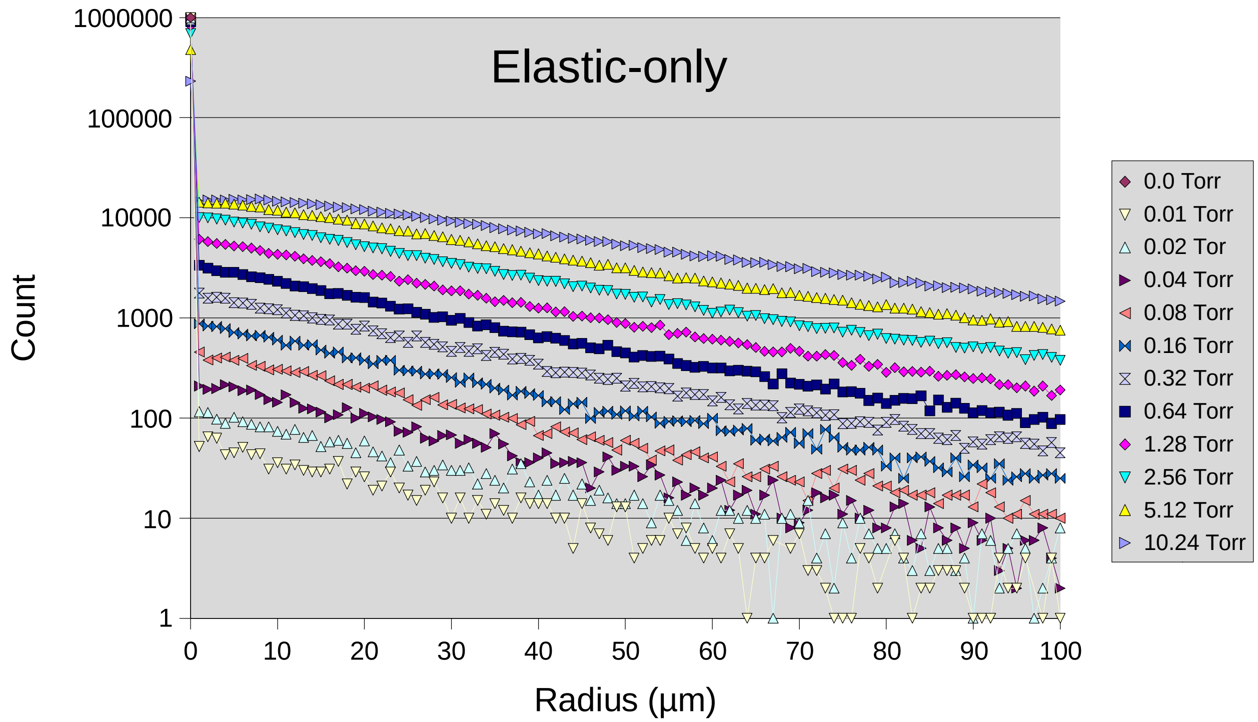
$$\sigma_i/\sigma_e \sim 20/Z$$

- Take the form of the differential cross section from Colliex & Mory 1984

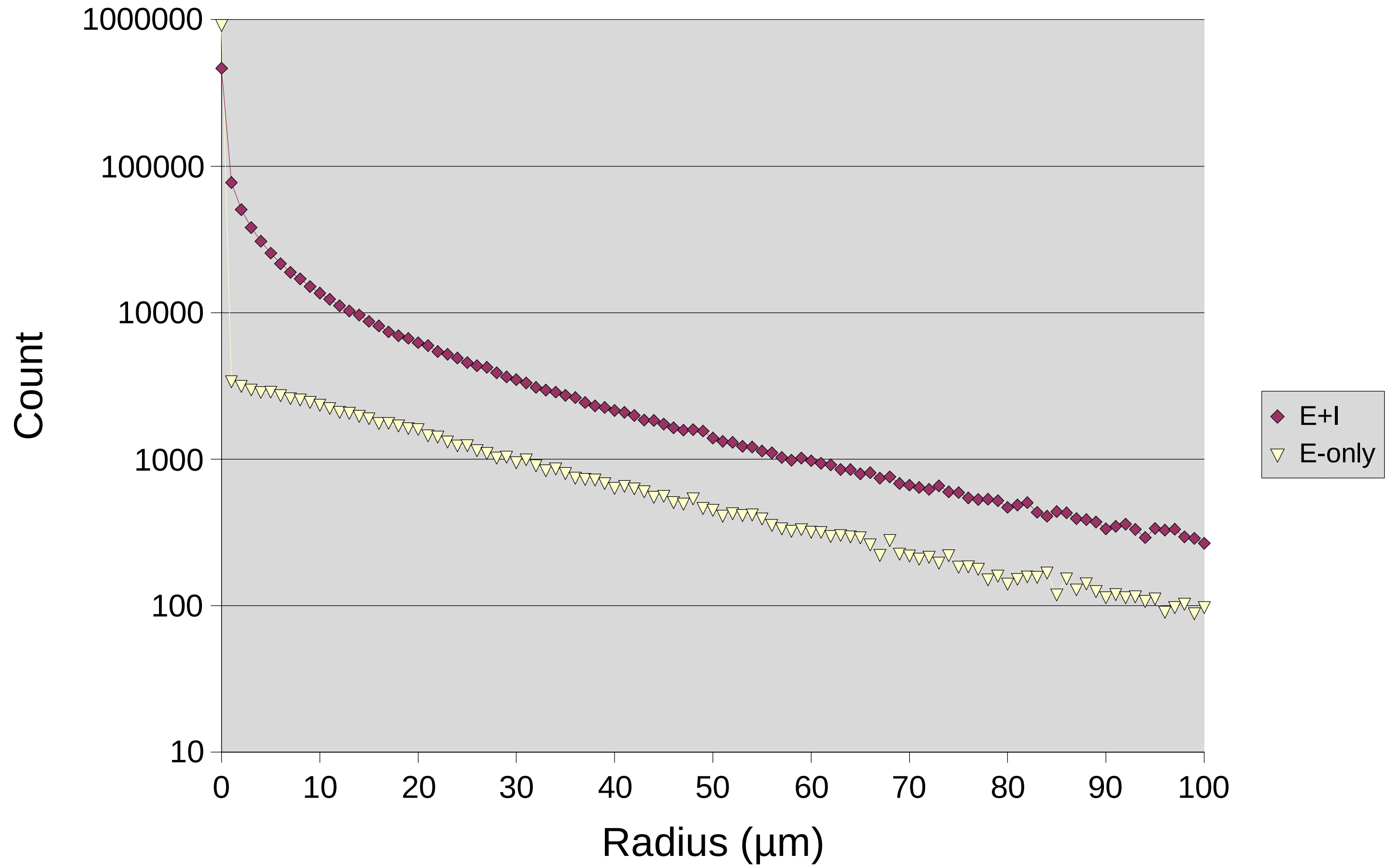
$$\frac{d\sigma_i}{d\Omega} = \frac{4\gamma^2 Z}{a_0{}^2 k_0{}^4} \frac{1}{(\theta^2+\theta_E{}^2)} \left\{ 1 - \left[\frac{\theta_0{}^4}{(\theta^2+\theta_E{}^2+\theta_0{}^2)^2} \right] \right\}$$

Egerton, R.F. , “Electron Energy-Loss Spectroscopy in the Electron Microscope”, second edition, Plenum Press, 1996
Colliex, C & Mory, C, in “Quantitative Electron Microscopy”, ed. J.N. Chapman & A.J. Craven,SUSSP Publications, Edinburgh


Elastic + Inelastic
Count
Radius (µm)
0
0.01 Torr
0.02 Tor
0.04 Torr
0.08 Torr
0.16 Torr
0.32 Torr
0.64 Torr
1.28 Torr
2.56 Torr
5.12 Torr
10.24 Torr

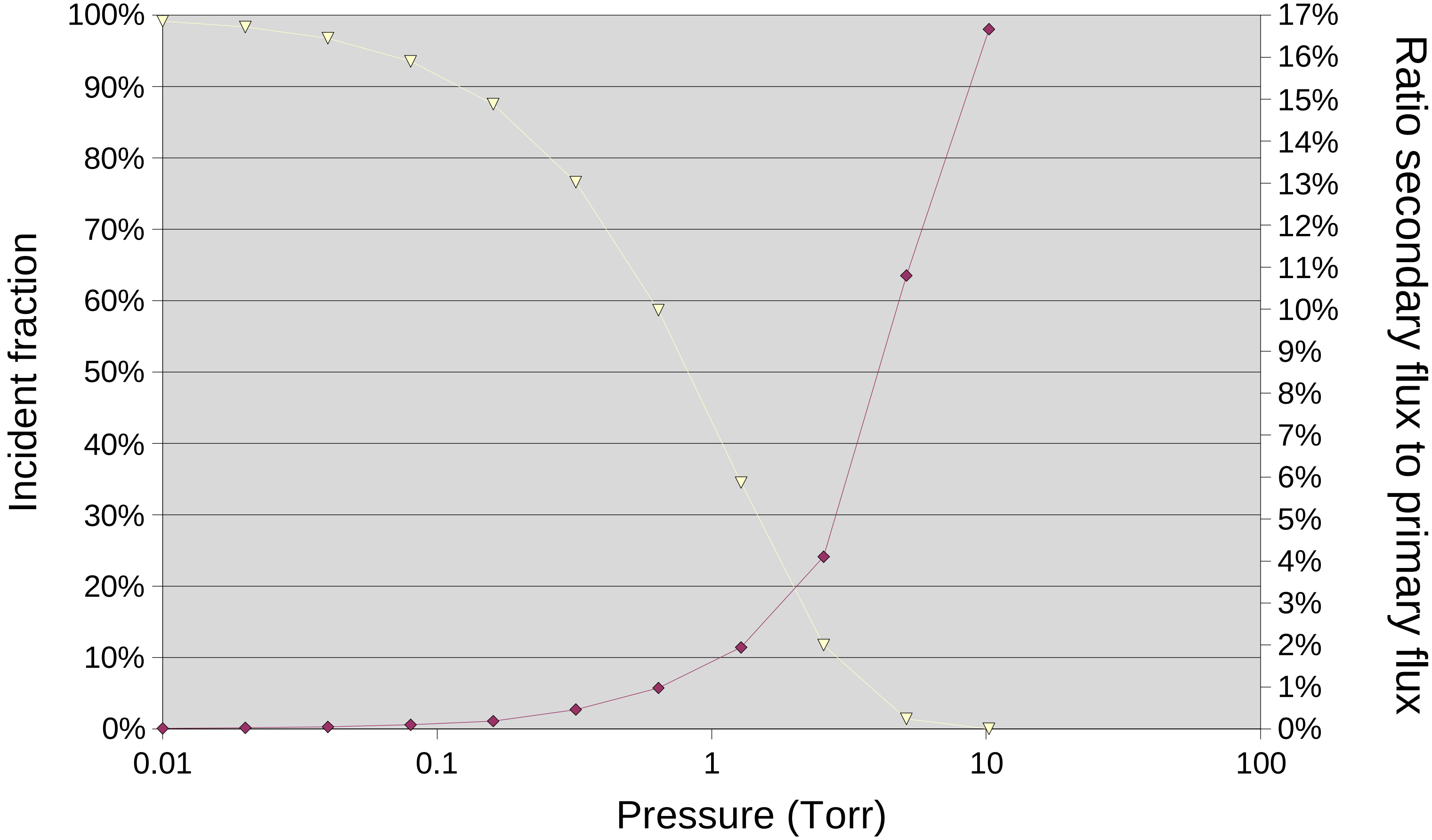

Elastic-only
Count
Radius (µm)
0.0 Torr
0.01 Torr
0.02 Tor
0.04 Torr
0.08 Torr
0.16 Torr
0.32 Torr
0.64 Torr
1.28 Torr
2.56 Torr
5.12 Torr
10.24 Torr

Comparing elastic and elastic+inelastic at 0.64 Torr of H_2O, 1 cm path

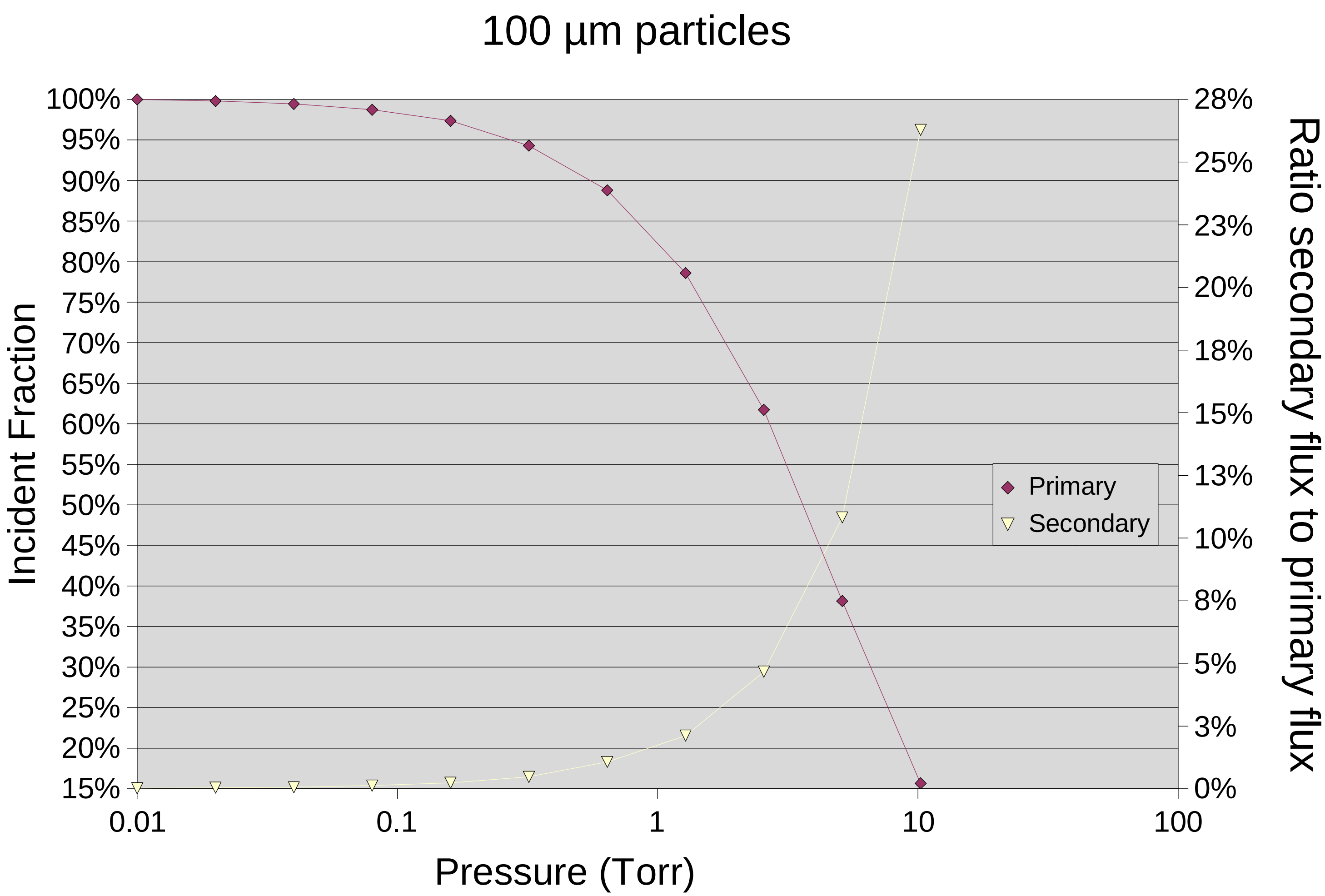


How much does an adjacent particle contribute to the spectrum?

Measure the ratio of the number of electrons striking the primary over the number of electrons striking the secondary.

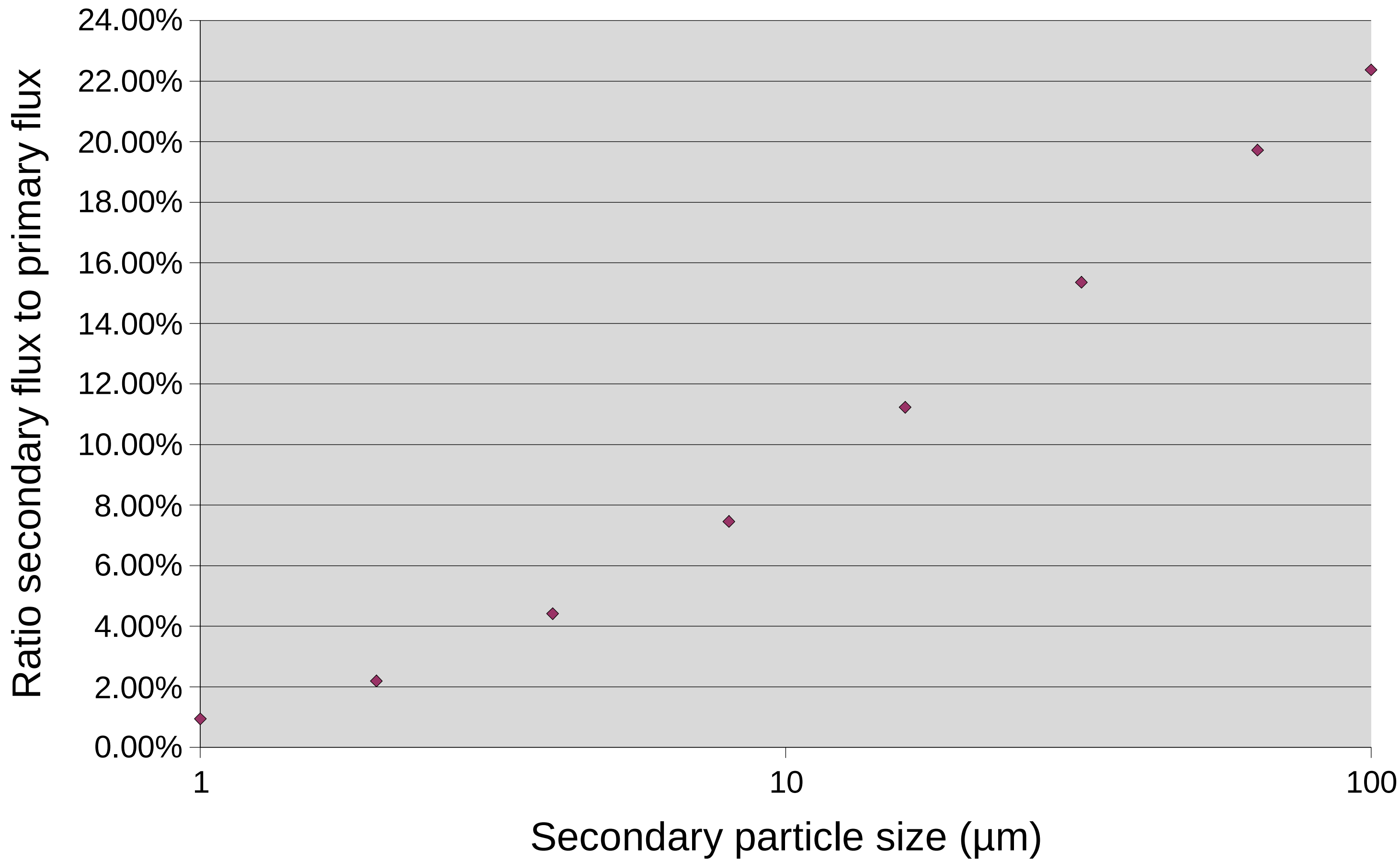


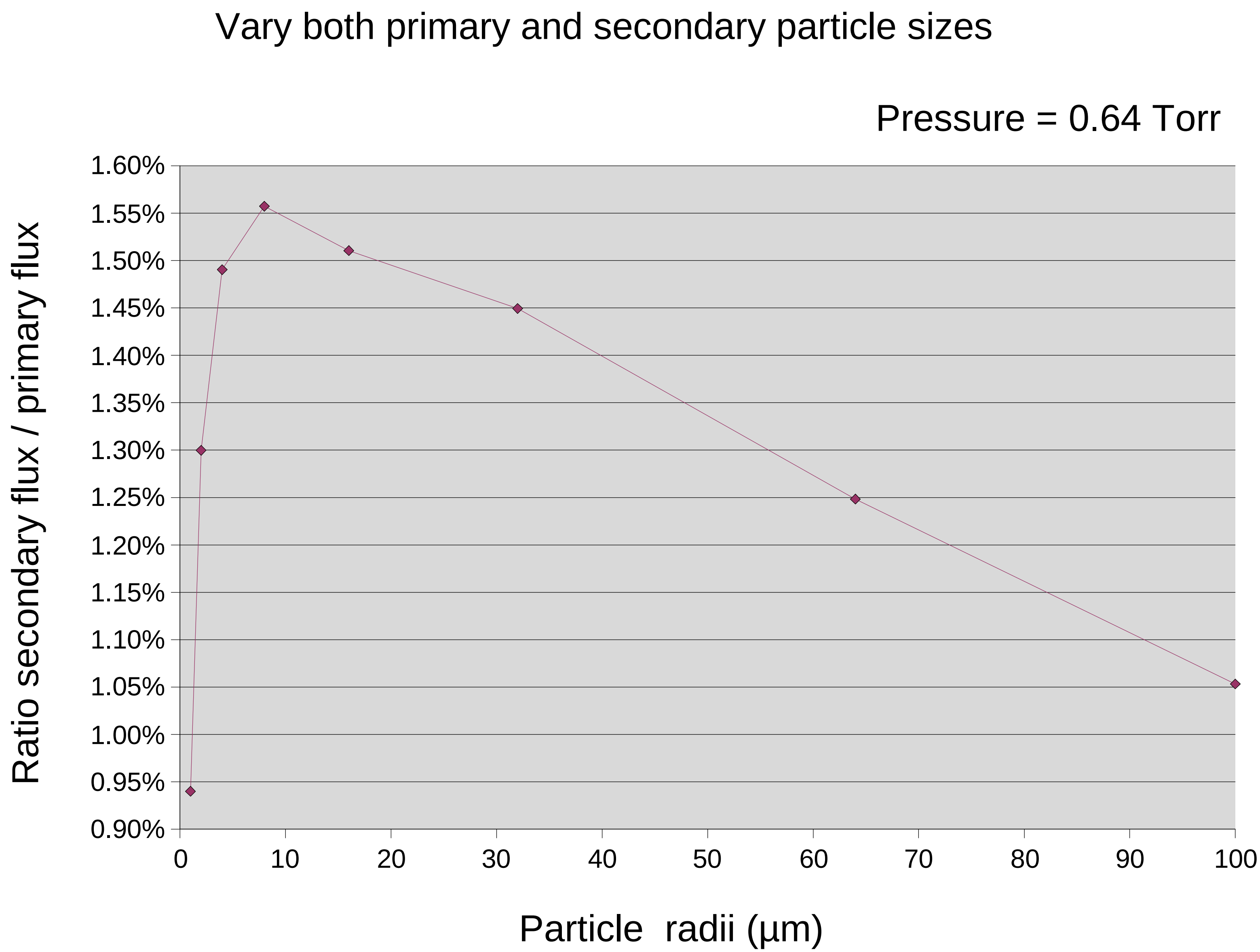
Two 1 µm adjacent particles, the beam centered on one.
1 cm path of H_2O vapor at the specified pressure



100 µm particles
Incident Fraction
Ratio secondary flux to primary flux
Pressure (Torr)
Primary
Secondary
100%
95%
90%
85%
80%
75%
70%
65%
60%
55%
50%
45%
40%
35%
30%
25%
20%
15%
28%
25%
23%
20%
18%
15%
13%
10%
8%
5%
3%
0%
0.01
0.1
1
10
100

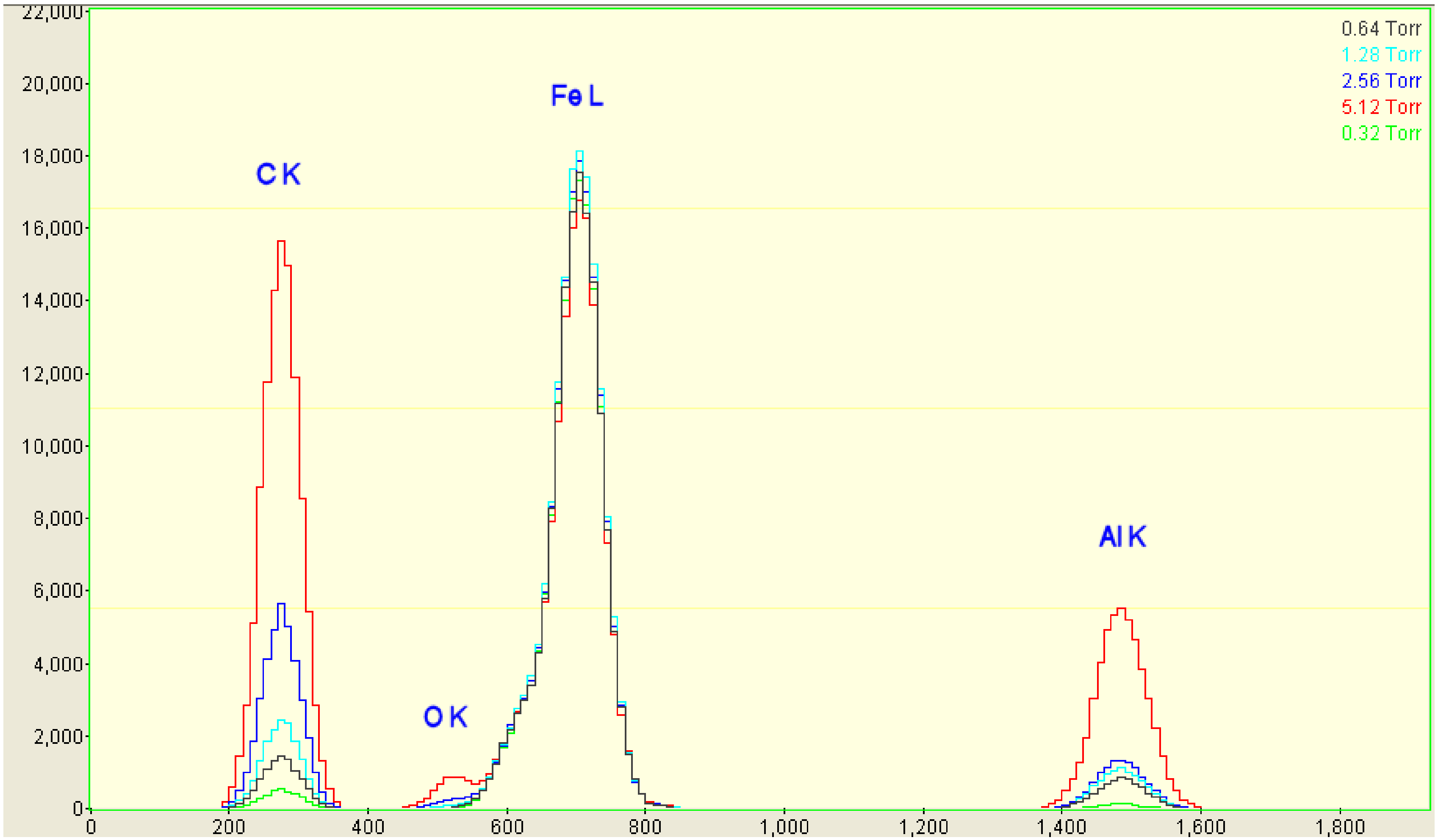
Keep the primary particle size 1 µm, vary the secondary particle size



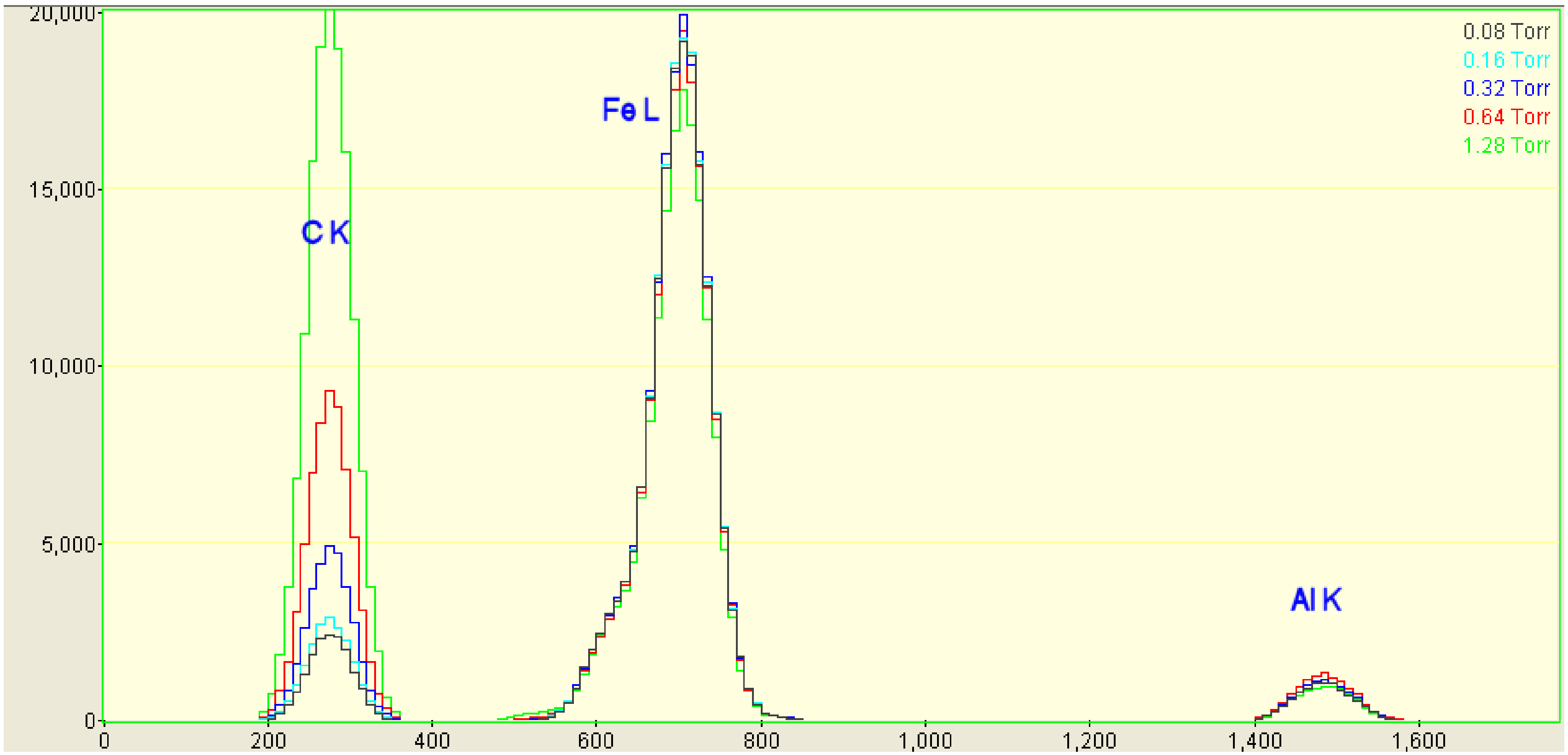


Vary both primary and secondary particle sizes
Pressure = 0.64 Torr
Ratio secondary flux / primary flux
1.60%
1.55%
1.50%
1.45%
1.40%
1.35%
1.30%
1.25%
1.20%
1.15%
1.10%
1.05%
1.00%
0.95%
0.90%
0
10
20
30
40
50
60
70
80
90
100
Particle radii (µm)

Modeled x-ray spectra from proximate 100 µm particles



Modeled x-ray spectra from proximate 1 µm particles

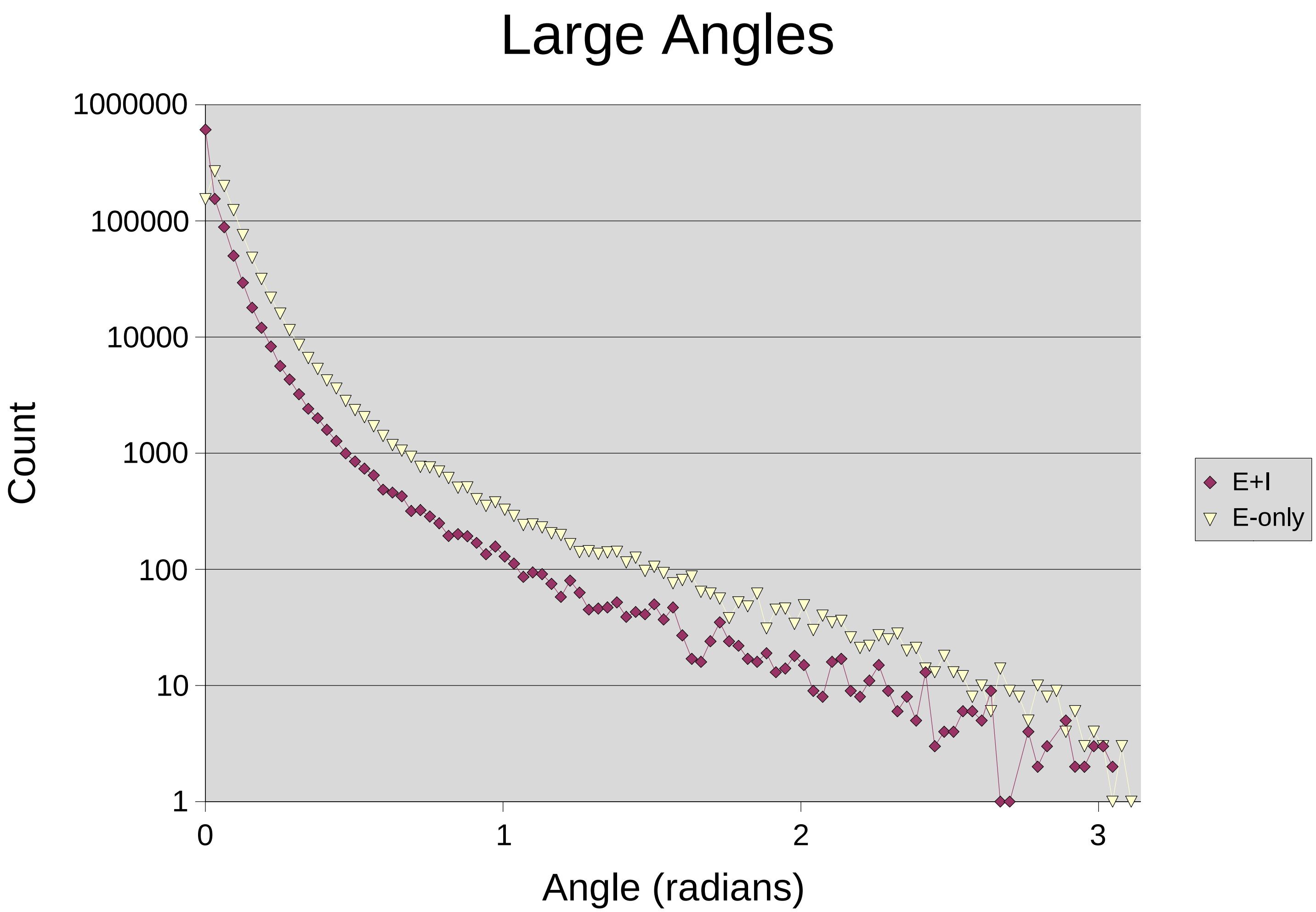


Remind me to show the VRML!

NISTMonte is currently available (with source) at

http://www.duck-and-cover.com

Comparing elastic and elastic+inelastic scattering



Comparing elastic and elastic+inelastic scattering